

Arclength Continuation and Bifurcation

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The objective of this chapter is to study parameter dependent nonlinear equations of the form

$$(0.1) \quad F(u, \lambda) = 0,$$

as the parameter λ varies. Here $u \in R^N$, λ is real, and $F : R^{N+1} \rightarrow R^N$.

In many cases the parameter λ has a physical meaning, representing a load, voltage drop, fluid velocity, or a chemical concentration, for example.

We will consider only scalar λ in this book, and will denote $\partial F/\partial \lambda$ by F_λ . The Jacobian matrix of F with respect to u will be denoted F_u .

Throughout this chapter we will assume that F is Lipschitz continuously differentiable.

There are many good books completely devoted to this topic, My favorite is [5], which focuses mostly on time-independent problems. For in-depth surveys of time-dependent problems see [3, 8]. The style of proofs in this chapter, like that of [5], is intended to be direct and specific, rather than maximally general.

We will work through some examples of differential and integral equations, and when we do that we will express things in terms of the continuous problem, not a discretization. Most of the time our conclusions for the continuous problem will also be valid for any sensible discretization. In infinite dimension, the derivative of a nonlinear map is not a Jacobian matrix, but rather a linear operator called the **Fréchet derivative**.

DEFINITION 0.1. *A nonlinear map F on a Banach space X is Fréchet differentiable at $x \in X$ if there is a bounded linear operator A on X such*

$$\lim_{\|w\| \rightarrow 0} \frac{\|F(x+w) - F(x) - Aw\|}{\|w\|} = 0.$$

The operator A is called the Fréchet derivative of F at x and is written $F'(x)$ or $F_x(x)$.

In finite dimension, if F has directional derivatives in all directions, then F is differentiable and one can construct the Jacobian by differentiating in the coordinate directions. In infinite dimension directional differentiability does not imply Fréchet differentiability. However, one usually computes a Fréchet derivative by expressing its action on an element of the space, *i. e.* computing a directional derivative. The formula for that is

$$F'(x)w = \left. \frac{\partial}{\partial \epsilon} F(x + \epsilon w) \right|_{\epsilon=0}.$$

We will only use the notion of Fréchet derivative for convenience, since Fréchet derivatives are easier to compute than the Jacobians of the discretized problem.

1. Parameter Continuation. **parameter continuation** is a simple approach that sometimes works quite well. The idea is to solve (0.1) for $\lambda = \lambda_{min}$, a parameter value for which the equation is easy to solve, say by Newton's method. Having computed (u_0, λ) , increment λ by a small value $d\lambda$, and use u_0 as the initial iterate for

$$(1.1) \quad F(u, \lambda + d\lambda) = 0.$$

Algorithm `paramc` is a simple realization of parameter continuation from λ_{min} to $\lambda_{max} = \lambda_{min} + n d\lambda$.

paramc($u, F, \lambda_{min}, d\lambda, n$)

Set $\lambda = \lambda_{min}, u_0 = u$

while $\lambda \leq \lambda_{max}$ **do**

Solve $F(u, \lambda) = 0$ with u_0 as the initial iterate to obtain $u(\lambda)$

$u_0 = u(\lambda)$

$\lambda \leftarrow \lambda + d\lambda$

end while

Algorithm `paramc` is too simple. One avenue for significant improvement is the choice of the initial iterate for the nonlinear solver. While using the result for the previous value of λ , as `paramc` does, can be effective, it would be more efficient, assuming that u is a smooth function of λ , to use several previously computed values of $u(\lambda)$ and extrapolate (think of predictor-corrector methods for initial value problems [1, 11]). This could allow one to use a larger $d\lambda$, and complete the continuation with less work. We will discuss issues like this in § 4.

2. The Implicit Function Theorem. The standard assumptions [6, 7] for Newton's method as applied to $F(u, \lambda) = 0$ are that a solution exists, that F_u , the Jacobian of F with respect to the vector u is Lipschitz continuous, and that $F_u(x(\lambda), \lambda)$ is nonsingular.

The **Implicit Function Theorem** states that existence of a solution at λ_0 , together with differentiability of F and nonsingularity of F_u , will imply existence of $x(\lambda)$ for λ near λ_0 , and also imply that $x(\lambda)$ is a smooth function of λ .

THEOREM 2.1. Implicit Function Theorem: *Let Ω be an open subset of R^{N+1} and let $F \in C^k(\Omega)$ for some integer $k > 0$. Assume that F_u and F_λ are Lipschitz continuous in Ω , the closure of Ω . Then if*

- $(u_0, \lambda_0) \in \Omega$,
- $F(u_0, \lambda_0) = 0$,
- $F_u(u_0, \lambda_0)$ is nonsingular,

then there are ρ and ϵ such that there is a unique solution

$$u(\lambda) \in \mathcal{B}_\rho(u_0) = \{u \mid \|u - u_0\| < \rho\}$$

of

$$F(u, \lambda) = 0$$

for all $\lambda \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon)$. Moreover $u \in C^k(\lambda_0 - \epsilon, \lambda_0 + \epsilon)$.

Proof. We will prove the existence part of the result with the contraction mapping theorem [6, 7] by finding ϵ and ρ such that the Newton map

$$\mathcal{T}(u) = \mathcal{T}(u, \lambda) = u - F_u(u_0, \lambda_0)^{-1}F(u, \lambda)$$

is a contraction on

$$\mathcal{B}_\rho(u_0) = \{u \mid \|u - u_0\| \leq \rho\}$$

if $\lambda \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon)$. Having done that, the contraction mapping theorem will imply that $u = \mathcal{T}(u, \lambda)$ has a unique solution in $\mathcal{B}_\rho(u_0)$.

We first reduce ρ and ϵ if necessary so that

$$\mathcal{N} = \{(u, \lambda) \mid \|u - u_0\| \leq \rho \text{ and } |\lambda - \lambda_0| \leq \epsilon\} \subset \Omega.$$

Let $u = u_0 + w$ and $\lambda = \lambda_0 + \mu$. The fundamental theorem of calculus and $F(u_0, \lambda_0) = 0$ imply that

$$(2.1) \quad \begin{aligned} F(u, \lambda) &= \int_0^1 F_u(u_0 + tw, \lambda_0 + t\mu)w \, dt + \int_0^1 F_\lambda(u_0 + tw, \lambda_0 + t\mu)\mu \, dt \\ &= F_u(u_0, \lambda_0)w + F_\lambda(u_0, \lambda_0)\mu + E(u, \lambda), \end{aligned}$$

where

$$(2.2) \quad \begin{aligned} E(u, \lambda) &= \int_0^1 \left(F_u(u_0 + tw, \lambda_0 + t\mu) - F_u(u_0, \lambda_0) \right) w \, dt \\ &\quad + \int_0^1 \left(F_\lambda(u_0 + tw, \lambda_0 + t\mu) - F_\lambda(u_0, \lambda_0) \right) \mu \, dt. \end{aligned}$$

From (2.2) we see that there is $C > 0$ such that if $u, v \in \mathcal{B}_\rho(u_0)$ and $|\lambda - \lambda_0| \leq \epsilon$ then

$$(2.3) \quad \|E(u, \lambda)\| \leq C(\epsilon + \epsilon\rho_0 + \rho_0^2)$$

and

$$(2.4) \quad \|E(u, \lambda) - E(v, \lambda)\| \leq C(\epsilon + \rho)\|u - v\|.$$

The constant C in (2.3) and (2.4) depends only on the Lipschitz constants of F_u and F_λ .

If $u \in \mathcal{B}_\rho(u_0)$ and $|\lambda - \lambda_0| \leq \epsilon$, then

$$(2.5) \quad \mathcal{T}(u, \lambda) = u_0 - F_u(u_0, \lambda_0)^{-1} \left(F_\lambda(u_0, \lambda_0)(\lambda - \lambda_0) + E(u, \lambda) \right)$$

and hence

$$\|\mathcal{T}(u, \lambda) - u_0\| \leq \|F_u(u_0, \lambda_0)^{-1}\| \left(\|F_\lambda(u_0, \lambda_0)\| \epsilon + C(\epsilon + \epsilon\rho_0 + \rho_0^2) \right) \leq \rho$$

if ρ and ϵ are sufficiently small. We have shown that N maps $\mathcal{B}_\rho(u_0)$ into itself if ρ and ϵ are sufficiently small.

To complete the proof of existence and uniqueness of u we must show that N is a contraction on $\mathcal{B}_\rho(u_0)$. That follows trivially from (2.4), since if $u, v \in \mathcal{B}_\rho(u_0)$, then

$$\|\mathcal{T}(u, \lambda) - N(v, \lambda)\| \leq C(\epsilon + \rho)\|F_u(u_0, \lambda_0)^{-1}\|\|u - v\| \leq \|u - v\|/2$$

for ϵ and ρ sufficiently small.

Our final task is to prove that u is a smooth function of λ . We will first show that u is a continuous function of λ for all $\lambda \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon)$. Let

$$\lambda_1, \lambda_2 \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon).$$

Let $u_j = u(\lambda_j)$, $\mu = \lambda_1 - \lambda_2$, and $w = u_1 - u_2$. Since $F(u_j, \lambda_j) = 0$ for $j = 1, 2$, we may apply the fundamental theorem of calculus and obtain

$$0 = F(u_1, \lambda_1) = F(u_2, \lambda_2) + \int_0^1 F_u(u_2 + tw, \lambda_2 + t\mu)w dt + \int_0^1 F_\lambda(u_2 + tw, \lambda_2 + t\mu)\mu dt.$$

Hence

$$(2.6) \quad F_u(u_0, \lambda_0)w = \int_0^1 \left(F_u(u_2 + tw, \lambda_2 + t\mu) - F_u(u_0, \lambda_0) \right) w dt + \int_0^1 F_\lambda(u_2 + tw, \lambda_2 + t\mu)\mu dt.$$

We must estimate the terms on the right side of (2.6). Let γ be the Lipschitz constant of F_u on $\bar{\Omega}$. Clearly

$$(2.7) \quad \left\| \int_0^1 \left(F_u(u_2 + tw, \lambda_2 + t\mu) - F_u(u_0, \lambda_0) \right) w dt \right\| \leq \|w\| \gamma \int_0^1 \|u_2 - u_0 + tw\| + t(\mu - \lambda_0) dt \leq \|w\| \gamma (\rho + \epsilon).$$

Continuity of F_λ on $\bar{\Omega}$ implies that

$$M = \max_{(u, \lambda) \in \bar{\Omega}} \|F_\lambda(u, \lambda)\| < \infty.$$

ence

$$(2.8) \quad \left\| \int_0^1 F_\lambda(u_2 + tw, \lambda_2 + t\mu)\mu dt \right\| \leq M|\mu|/2.$$

Combining (2.7), (2.8), and the nonsingularity of $F_u(u_0, \lambda_0)$ implies

$$\|w\| \leq \|F_u(u_0, \lambda_0)^{-1}\| (\gamma(\rho + \epsilon)\|w\| + M|\mu|/2).$$

Hence for ρ and ϵ sufficiently small,

$$\|w\| \leq \frac{\|F_u(u_0, \lambda_0)^{-1}\| M|\mu|/2}{1 - \|F_u(u_0, \lambda_0)^{-1}\| \gamma(\rho + \epsilon)} = O(|\mu|),$$

which proves continuity of u as a function of λ .

The remaining part of the proof is the verification of differentiability. If one formally differentiates $F(u, \lambda) = 0$ with respect to λ one obtains

$$F_u \frac{du}{d\lambda} + F_\lambda = 0$$

and hence

$$\frac{du}{d\lambda} = -F_u^{-1} F_\lambda.$$

We will prove that this formal manipulation is rigorous.

Let

$$\lambda_1, \lambda_2 \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon),$$

we showed above that

$$\begin{aligned} 0 &= F(u(\lambda_2), \lambda_2) \\ &= F(u(\lambda_1), \lambda_1) + F_u(u(\lambda_1), \lambda_1)(u(\lambda_2) - u(\lambda_1)) + F_\lambda(u(\lambda_1), \lambda_1)(\lambda_2 - \lambda_1) \\ &\quad + O(|\lambda_2 - \lambda_1|^2) \\ &= F_u(u(\lambda_1), \lambda_1)(u(\lambda_2) - u(\lambda_1)) + F_\lambda(u(\lambda_1), \lambda_1)(\lambda_2 - \lambda_1) + O(|\lambda_2 - \lambda_1|^2). \end{aligned}$$

Hence

$$\frac{u(\lambda_2) - u(\lambda_1)}{\lambda_2 - \lambda_1} = -F_u(u(\lambda_1), \lambda_1)^{-1} F_\lambda(u(\lambda_1), \lambda_1) + O(|\lambda_2 - \lambda_1|),$$

and, therefore,

$$(2.9) \quad \frac{du(\lambda)}{d\lambda} = -F_u(u(\lambda), \lambda)^{-1} F_\lambda(u(\lambda), \lambda).$$

We may continue to differentiate (2.9) with the chain rule as long as F supports the differentiation. This (at last!) completes the proof.

□

2.1. Success and Failure of Parameter Continuation. If F_u were nonsingular for all problems, this discussion would be over, because the implicit function would tell us that we could continue with a given fixed step size $d\lambda_{min}$ for as long as we liked.

2.1.1. Example: Failure of Parameter Continuation. One can not consistently depend on the nonsingularity of F_u . As an example we use the Chandrashekar H-equation [2, 6, 10] and compute

$$\|H\|_1 = \int_0^1 H(\nu, c) d\nu$$

as a function of the parameter c . We write the equation as

$$H(\mu) = 1 + \frac{c}{2} H(\mu) \int_0^1 H(\nu) \frac{d\nu\mu}{\mu + \nu}$$

and integrate with respect to μ . One gets

$$\|H\|_1 = 1 + \frac{c}{2} \int_0^1 \int_0^1 \frac{H(\mu)H(\mu)\mu d\mu d\nu}{\mu + \nu} = 1 + \frac{c}{4} \|H\|_1^2,$$

and so

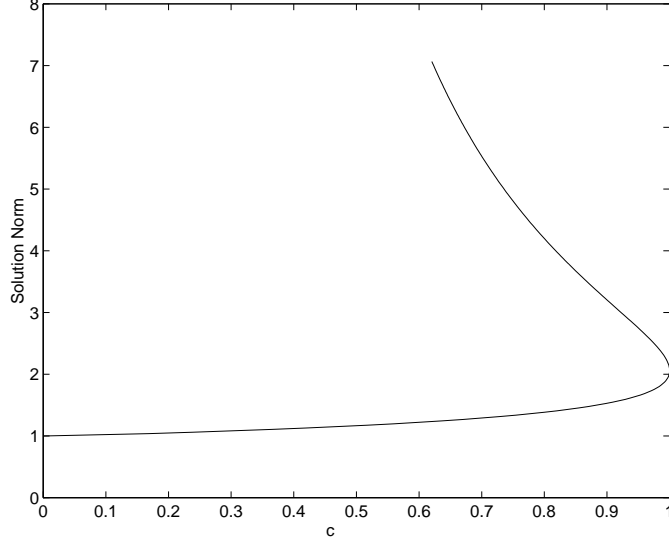
$$(2.10) \quad \|H\|_1 = \frac{1 \pm \sqrt{1 - c}}{c/2}.$$

Equation (2.10) tell us two interesting things. First, there can be no real solutions of the H equation for $c > 1$, so there must be a singularity at $c = 1$, or the implicit function theorem would

tell us that we could continue past $c = 1$. Secondly, the \pm gives us a hint that there may be two solutions, at least for $0 < c < 1$ (and there are!).

Figure 2.1 is a plot of $\|H\|_1$ against λ . In § 3 we will explain how we made the plot, but for now simply notice how the curve bends around when $c = 1$, and how there are two solutions for each $0 < c < 1$.

FIG. 2.1. $\|H\|_1$ as a function of c



In the particular case of the H equation, it's possible to compute the singularity analytically. Write the H equation as

$$F(H, c)(\mu) = H(\mu) - \left(1 - \frac{c}{2} \int_0^1 \frac{\mu H(\nu) d\nu}{\mu + \nu}\right)^{-1}.$$

Taking the Fréchet derivative of F in the direction of w yields

$$F_H(H, c)w(\mu) = w(\mu) - \frac{\frac{c}{2} \int_0^1 \frac{\mu w(\nu) d\nu}{\mu + \nu}}{\left(1 - \frac{c}{2} \int_0^1 \frac{\mu H(\nu) d\nu}{\mu + \nu}\right)^2} = w(\mu) - \frac{c}{2} H(\mu)^2 \frac{c}{2} \int_0^1 \frac{\mu w(\nu) d\nu}{\mu + \nu}.$$

Let $c = 1$, then (2.10) implies that

$$\int_0^1 H(\mu) d\mu = 2$$

and therefore

$$\begin{aligned} \frac{1}{2} \int_0^1 \frac{\nu H(\nu) d\nu}{\mu + \nu} &= \frac{1}{2} \int_0^1 H(\nu) \left(1 - \frac{\mu}{\mu + \nu}\right) d\nu \\ &= 1 - \int_0^1 \frac{\mu H(\nu) d\nu}{\mu + \nu} \\ &= 1 - H(\mu)^{-1} \end{aligned}$$

Hence if $\phi(\mu) = \mu H(\mu)$,

$$F_H(H, 1)\phi = 0,$$

and we have shown directly that F_H is singular at $c = 1$.

More can be done, one can apply the Perron-Frobenius theory [4,9] to show that the null space of F_H has dimension one, and hence is spanned by ϕ . We will show in § 3 how the singularity can be resolved in a simple way because

$$F_c(H, 1) = H^2(H^{-1} - 1) = H - H^2$$

is not in the range of F_H .

3. Pseudo-arclength Continuation. The curve in Figure 2.1, has no self-intersections. If we were to parameterize that curve with respect to arclength and use the arclength s as a parameter, we could draw the curve using simple parameter continuation, where $x = (u, \lambda)^T$ would play the role of u and s would be the parameter.

The new **extended equations** have form

$$(3.1) \quad G(x, \lambda) = \begin{pmatrix} F(u, \lambda) \\ N(u, \lambda, s) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The **normalization equation** $N = 0$ is an approximation to the statement that s represents arclength.

If we let \dot{x} denote differentiation with respect to s then, keeping in mind that we are using the Euclidean norm in all dimensions, we have

$$(3.2) \quad \|\dot{x}\|^2 = \|\dot{u}\|^2 + |\dot{\lambda}|^2 = 1$$

says that s is arclength. Practical methods approximate (3.2), and hence are given the name of **pseudo-arclength continuation**.

Any normalization will either approximate or compute \dot{x} and use one or more known points on the path. For example, if one has computed a current point $x_0 = (u_0^T, \lambda_0)^T$ and a approximation to \dot{x}_0 , one could use

$$(3.3) \quad N(x, s) = \dot{x}_0^T(x - x_0) - (s - s_0) = 0$$

which is an approximation to (3.2).

We could use this normalization in the following way. Given x_c and a step in arclength $ds = x - x_0$, we might solve (3.1) with the normalization given by (3.3) with Newton's method using x_0 as the initial iterate. If the singularities in the path are no worse than the one for the H-equation, this is a reasonable method if ds is sufficiently small and one does not require a segment of the solution path that is too long.

Algorithm `psarc` is a simple implementation of pseudo-arclength continuation, and is little more than parameter continuation as applied to G , rather than F , with s as the parameter.

arc_simple($u, F, \lambda_{min}, d\lambda, s_{max}$)

Set $s = 0, \lambda = \lambda_{min}, x_0 = (u^T, \lambda)^T$

while $s < s_{max}$ **do**

 Approximate \dot{x}

 Solve $G(x, s) = 0$ with x_0 as the initial iterate obtain $x(s)$.

$x_0 = x(s)$

$s \leftarrow s + ds$

end while

4. Implementation Details. A practical algorithm must pay attention to,

- the approximation of \dot{x} ,
- the **predictor**, *i. e.* the construction of a good initial iterate for the Newton iteration at the next point on the path,
- changing ds in response to the curvature of the path or the performance of the nonlinear solver, and
- effective use of the structure of the problem.

We will discuss these issues in the sections that follow.

4.1. Computation of \dot{x} .

4.1.1. Analytic Computation of \dot{x} . If F_u is nonsingular, one can compute \dot{x} exactly. We begin by differentiating $F(u, \lambda) = 0$ with respect to s to get

$$F_u \dot{u} + F_\lambda \dot{\lambda} = 0$$

and obtain

$$(4.1) \quad \dot{u} = -F_u^{-1} F_\lambda \dot{\lambda}.$$

Keep in mind that $\dot{\lambda}$ is a scalar. We can compute $|\dot{\lambda}|$ by using (3.2) and (4.1) to obtain

$$\|\dot{x}\|^2 = \|\dot{u}\|^2 + |\dot{\lambda}|^2 = \dot{\lambda}^2 (\|F_u^{-1} F_\lambda\|^2 + 1) = 1.$$

Hence

$$|\dot{\lambda}| = (\|F_u^{-1} F_\lambda\|^2 + 1)^{-1/2}.$$

The only thing remaining is to compute the sign of $\dot{\lambda}$. This is an important thing to do correctly, for if we get the sign wrong, we could recomputed the path in the direction we came from. Keeping the sign of $\dot{\lambda}$ constant, *i. e.* the same sign as the difference in λ of the first two points on the path, is perfectly save. The sign of $\dot{\lambda}$ will change only at a point where $\dot{\lambda} = 0$. At such a point, (4.1), if valid, would imply that $\dot{u} = 0$, which would violate (3.2). The resolution of this is that if $\dot{\lambda} = 0$, then F_u must be singular.

Get something in here about getting the sign of $\dot{\lambda}$ right after a singularity has been passed.

4.1.2. Secant Approximation of \dot{x} . If we have computed two points on the path $x_{-1} = x(x_{-1})$ and $x_0 = x(s_0)$, we can use the approximation

$$\dot{x} = Dx \|Dx\|$$

where

$$Dx = \frac{x_0 - x_{-1}}{s_0 - s_{-1}},$$

in (3.3). If one does this, the one must initialize the continuation with two solutions (u_i, λ_i) , $i = -1, 0$, of $F(u, \lambda) = 0$, and then estimate $s_0 - s_{-1}$ by

$$s_0 - s_{-1} = \sqrt{\|u_0 - u_{-1}\|^2 + (\lambda_0 - \lambda_{-1})^2}.$$

4.2. The Predictor. One easy choice for an initial iterate, and the choice used in Algorithm `arc_simple` is to initialize the nonlinear iteration with the x_0 the previously computed point on the path. This **trivial predictor** can, and often does, work well, but it does not use all the information at hand. The **tangent predictor**, uses the knowledge of \dot{x} at s_0 to build a higher order predictor

$$x_{tan} = x_0 + \dot{x}(s - s_0).$$

If the path is smooth, then the trivial predictor is a first order (in $ds = s - s_0$) accurate approximation to the solution $x(s)$ and the tangent predictor is second order accurate. If one has computed several points on the path, a high-order polynomial predictor could also be used.

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